1. **Project Name:** **Development of Semi-Stochastic Algorithm for Optimizing Alloy Composition of High-Temperature Austenitic Stainless Steels (H-Series) for Desired Mechanical and Corrosion Properties**

2. **Lead Organization:** The University of Texas at Arlington
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3. **Principal Investigator:**
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4. **Project Partners:**

Type	Organization	Investigator	Responsibilities
DOE National Laboratory	ORNL	Vinod K. Sikka Peter Angelini	Conduct all aspects of melting, casting, and processing of the chosen alloy composition in support of data input and verification of results of semi-stochastic model.
Steel Producer	Duraloy Technologies, Inc.	Roman Pankiw	Will assist with requirements and limitations of certain alloy compositions to standard melting and casting procedures.
Steel User	Bethlehem Steel Corporation	Tony Martocci	Will assist in identifying property requirements for their applications.
Steel/Heat-Treating User	The Timken Company	Mark Carlson	Will assist in identifying property requirement for their applications.
Steel/Chemical/Heat Treating	Edison Industry of Ohio	Robert Purgert	Will assist in identifying property requirement for their applications and testing of components.

5. **Date Project Initiated and FY of Effort:** 01/01/2002 FY2003

6. **Expected Completion Date:** 12/31/04

7. Project Technical Milestones and Schedule:

Identification Number	Task / Milestone Description	Planned Completion Date	Actual Completion Date	Comments
1	**Development of Initial Plan of Experiment**	1/1/02-3/31/02	3/31/02	Completed on schedule
1.1	Generate alloy compositions with only six elements	1/1/02-6/31/02	6/30/02	Completed on schedule
1.2	Generate alloy compositions with 7 to 16 elements	1/1/02-9/31/02	9/30/02	Completed on schedule
2	**Analysis of the Plan of Experiment, Identification of the Objective Functions and Objective Constraints**	1/1/02-03/31/02	3/31/02	Completed on schedule
2.1	Objective to identify will include tensile, creep, and corrosion data	1/1/02-12/31/02	12/31/02	Completed except for corrosion
2.2	Objective constraints will include the acceptable number of alloying elements and use temperature and time	1/1/03-12/31/04	12/31/02	Completed except for time
3	**Determine Solution of M Particular Optimization Problems for Objective Constraints Defined in Task 2**	1/1/02-12/31/04		On schedule
3.1	Determine solutions for tensile properties	1/1/02-12/31/02	12/31/02	Completed on schedule
3.2	Determine solutions for tensile and creep properties	10/1/02-12/31/03		On schedule
3.3	Determine solutions for tensile, creep, and corrosion properties	10/1/03-12/31/04		
4	**Experimental Verification and Identification of Additional Experiments Needed**	10/1/02-12/31/04		
4.1	Complete experimental verification of tensile solution	10/1/02-12/31/04		
4.2	Complete experimental verification of tensile and creep solutions	7/1/03-12/31/04		
4.3	Complete experimental verification of tensile, creep, and corrosion properties	4/1/04-12/31/04		
5	**Prepare Alloys and Develop Tensile, Creep, and Corrosion Data**	1/1/02-12/31/04		
5.1	Test alloys for tensile properties	1/1/02-12/31/02		
5.2	Test alloys for creep properties	1/1/02-12/31/04		
5.3	Test alloys for corrosion properties	1/1/02-12/31/04		
6	**Meeting and Technical Reports**	1/1/02-12/31/04		
6.1	Hold one technical meeting each year	1/1/02-12/31/04	11/06/02	Meeting held at ORNL
6.2	Complete final report	1/1/02-12/31/04	03/28/03	On schedule

8. Past Project Milestones and Accomplishments:

We have licensed a basic version of the semi-stochastic multi-objective optimization software from IOSO in Moscow, Russia. This software is the result of over 20 years of research and development of its creator, Dr. Igor N. Egorov. The agreement with Dr. Egorov was that he will visit UTA at least once every year and spend at least one week working with Prof. George S. Dulikravich on modifications of the basic software so that it can perform the research tasks proposed in this project. Dr. Egorov visited UTA during Dec. 14-28, 2001 and delivered the basic version of IOSO software. He again visited UTA during September 7-14, 2002. He communicated with Prof. Dulikravich via e-mail regularly and provided advice on modifications needed in his basic IOSO optimization software.

Initially, Dr. Vinod K. Sikka from ORNL has defined a preliminary set of nine experimental data on rupture strength and tensile strength of H-series steels. We ran the IOSO optimizer on this problem, but results were unacceptably poor because of the very large number of design parameters (there were 14 alloying elements in these data sets) and an inadequately small number of experimental data sets available (there were only 9 data sets). In other words, there was not enough data for initial training of a special version of artificial neural network that is one of the modules in the IOSO package.

Dr. Vinod K. Sikka then provided a publicly available set of seventeen experimental data for rupture strength of H-series steel after 100 hours at temperature of 1800 F. Based on the concentration values of the six most important ingredients, we specified their minimum and maximum values. We then ran the modified IOSO optimizer on this problem, and obtained the first generation of optimized concentrations of alloys. Our presentation at the DOE Symposium in Albuquerque, NM, July 7-8, 2002 was converted into a technical paper and submitted for presentation in the Yazawa Symposium at the Annual TMS Meeting, San Diego, CA, March 5-8, 2003. Dr. Vinod K. Sikka then compiled a set of 201 experimental data for rupture strength of H-series steel with different life spans at different temperatures. Based on the concentration values of the 17 most important ingredients, we specified their minimum and maximum values for the optimization purposes as 10 percent below and above these values, respectively. Three simultaneous objectives were also defined: maximize the alloy life (HOURS), maximize the operating temperature (TEMP), and maximize the operating stress (PSI). The original experimental data set was reduced to a more coherent dataset by eliminating those data points that were clearly significantly outside of the typical range. The reduced data set had 158 data points. We then ran the modified IOSO optimizer on this problem, and obtained Several Pareto fronts. A more economical approach was also utilized where two-objective optimization (maximize PSI and maximize HOURS) for several operating temperature ranges was performed.

In early September of 2002, Prof. Igor N. Egorov visited Prof. Dulikravich at UTA and worked with him on explaining certain aspects of his IOSO optimization software. In early November of 2003, Prof. Dulikravich visited Dr. Sikka at ORNL and presented a lecture on the preliminary results of multi-objective optimization of high-temperature steel alloys. A number of researchers from ORNL met with Prof. Dulikravich. Very useful suggestions were made on how to modify this research and what types of results would be the most useful to materials designers. Specifically, the appropriate ranges for percentages of each of the most important chemical species in typical H-series steel were established and the original list of chemical species whose percentages were optimized was reduced to a more appropriate smaller number. Dr. Sikka's team provided a large set of experimental data for rupture strength of H-series steel with different life spans at different temperatures. Based on the concentration values of the most important ingredients, we specified their minimum and maximum values for the optimization purposes. Three simultaneous objectives were also defined: maximize the alloy life until rupture (HOURS), maximize the operating temperature (TEMP), and maximize the operating stress

(PSI). The original experimental data set was reduced to a more coherent dataset by eliminating those data points that were incomplete, duplicate, or significantly outside of the typical range. We then ran the modified IOSO optimizer on this problem, and obtained several Pareto fronts. A more economical approach was also utilized where two-objective optimization (maximize PSI and maximize HOURS) for several operating temperature ranges was performed. Following the suggestions from ORNL, we also ran test cases where only nine and only eight ingredients were optimized in the given reduced experimental data set. The objective was to see how different the optimization results will be for such smaller number of ingredients. As expected, lowering the number of design variables (chemical species whose percentages need to be optimized) for a given set of experimental data that was obtained for a significantly larger number of the ingredients has caused the optimization results to deteriorate. This was expected because of the significantly reduced number of options (number of ingredients) that were asked to create alloys with performance that is superior to the existing alloys that used a large number of obviously influential ingredients. Sensitivities of the three objectives to the variation in each of the alloying elements were also obtained for a number of optimized alloys (Pareto front points).

9. Planned Future Milestones:

1. Define the most appropriate additional optimization objectives including analytical definitions of the corrosion resistant alloys performance.
2. Search for a more uniform and coherent set of experimental data available from published sources.
3. Define the number of design parameters (alloying elements) that is the most appropriate for an available experimental data set size.
4. Compare the predicted properties of the optimized alloy compositions against the remaining part of the publicly available experimental data sets.
5. Define optimized concentrations for an appropriate minimum number of new alloys that will be created and experimentally tested in order to definitively confirm the validity of the entire methodology.
6. Determine a set of optimized alloys for tensile and creep properties.
7. Test predicted optimized alloys for tensile and creep properties.

10. Issues/Barriers:

The main barrier to even faster progress on this project has been the size of the available experimentally obtained data set of physical properties and chemical compositions of H-series steels. Even when such data sets eventually became available, a high degree of non-reliability of many of these data made the usable part of such data sets much smaller than the originally provided. Furthermore, these experimental data were obviously obtained at different facilities at different times and, apparently, not always under the same conditions. The current data set that we have seems to be satisfactory for the purpose of performing the proposed research, but it is strongly recommended that an organized effort is funded for establishing a reliable data bank for experimental data of high quality steel alloys.

11. Intended Market and Commercialization Plans/Progress:

There has been an excellent progress on developing a commercial quality software package for the optimization of several physical properties of H-series steel alloys, that is, of determining concentration of each chemical element in such alloys. Since accuracy of experimental evaluation of concentration of each chemical element in an alloy and the accuracy of manufacturing an alloy with the specified optimized chemical composition will affect the results of the optimization process, the software is now being modified to include some elements of the uncertainty level of the experimentally obtained data. The final software package is expected to become available for commercial dissemination to US steel manufacturers by the end of 2003.

12. Patents, publications, presentations:

1. Regular communications between Prof. George S. Dulikravich (UTA) and Dr. Vinod K. Sikka (ORNL) and Dr. Igor N. Egorov (IOSO Center) have been maintained via e-mail and telephone.
2. Professor Dulikravich presented the preliminary findings at the DOE IMF Workshop in Albuquerque, NM, July 5-7, 2002.
3. Professor Dulikravich presented an up-to-date set of results at the ORNL on November 7, 2002 (Attachment 2).
4. Professor Dulikravich presented an up-to-date set of results at the UTA's Department of Mathematics in March of 2003.
5. Professor Dulikravich presented a technical paper entitled "Semi-Stochastic Optimization of Chemical Composition of High-Temperature Austenitic Steels for Desired Mechanical Properties", by Dulikravich G. S., Egorov, I. N., Sikka, V. K. and Muralidharan, G. at the Yazawa Symposium, 2003 TMS Annual Meeting, San Diego, CA, March 2-6, 2003.

Highlight

This project deals with industry-wide need for improving material property performance for the applications that they are currently used for and to increase their upper use temperature for applications that improve the process efficiencies such as chemical and hat-treating processes carried out at higher than currently used temperatures. The proposed project takes a new approach of using stochastic optimization algorithm for optimizing alloy properties with minimum number of experimental evaluations of the candidate alloys. The proposed approach has the potential of identifying new compositions that cannot be identified without carrying out thousands of experiments. Furthermore, the approach has the potential for creating and designing alloys for each application, thereby maximizing their utilization at reduced cost.

The key to the success of the proposed research is the robustness, accuracy, and efficiency of the proposed multi-objective constrained optimization algorithm. There are only a few commercially available general-purpose optimization software packages. They all use almost exclusively a variety of standard gradient-based optimization algorithms, which are known to be unreliable because of their tendency to terminate in the nearest feasible minimum instead of finding a global optimum. Moreover, these optimizers can perform only optimization of a weighted linear combination of objective functions. This formulation does not provide a true multi-objective optimization capability, that is, each individual objective is not fully maximized. These optimizers require an extremely large number of objective function (mechanical and corrosion properties of alloys) evaluations, which makes the total number of experimental evaluations unacceptably large.

However, semi-stochastic truly multi-objective constrained optimization algorithms have not been commercialized yet and have not been demonstrated in this field of application. The proposed research is based on the use and a special adaptation of a new stochastic optimization algorithm specifically for the task of optimizing properties of alloys while minimizing the number of experimental evaluations of the candidate alloys. The proposed multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. Both weighted linear combination of several objectives and true multi-objective formulation options creating Pareto fronts are incorporated in the algorithm. The main benefits of this algorithm are its outstanding reliability in avoiding local minimums, its computational speed, and a significantly reduced number of required experimentally evaluated alloy samples as compared to more traditional semi-stochastic optimizers like genetic algorithms. Furthermore, the self-adapting response surface formulation used in this project allows for incorporation of realistic non-smooth variations of experimentally obtained data and allows for accurate interpolation of such data.

The basic version of the licensed semi-stochastic multi-objective optimization software called IOSO was augmented so that now it can handle up to 17 design variables (alloying elements). We ran the updated IOSO optimizer on a new large data set by optimizing simultaneously three physical properties while taking into account either 8, 9, 11, 14 or 17 alloying elements. The results were very educational demonstrating clearly that by involving more alloying elements the properties of the H-series steel can be significantly improved.